Effet of instrument sensitivity on relationships between total-column δD and precipitable water

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Supplementary material for "The role of continental recycling in intra-seasonal variations of continental moisture as deduced from model simulations and water vapor isotopic measurements" by Risi et al.

1 Goal

In the paper, we discuss the relationships between column-integrated δD and precipitable water (W), as observed by GOSAT and TES and as simulated by the LMDZ model. Remote sensing retrievals of water isotopic composition are however complex, and several effects may affect the observed relationships and the model-data comparison.

1. The data has limited vertical resolution. In addition, strong a-priori constraints can significantly distort the retrievals. These effects may depend on the water content of the atmosphere, and thus they may affect δD-W relationships. The effects of limited vertical resolution and a-priori constraints are described by the averaging kernels.

2. When comparing the model to the data, the sensitivity of the measurement (limited vertical resolution, strong a-priori constraints) needs to be taken into account. This is done by applying averaging kernels to the model outputs. However, model biases in humidity may affect the model-data comparison of column-integrated δD. For example, model biases in upper-tropospheric humidity may be propagated to the lower-tropospheric δD through the averaging kernels (e.g. [Worden et al., 2012]).

The goal of this supplementary material is to quantify the influence of these two effects on the interpretation of observed δD-W relationships and of model-data differences in these relationships.

1. To quantify the influence of limited vertical resolution and a-priori constraints on observed δD , we compare total-column δD simulated with LMDZ and total-column δD obtained after convolution with the averaging kernels, assuming that simulated humidity profile equals the a-priori humidity profile, as justified in section 2.

2. To quantify the influence of model biases in humidity on the model-data comparison of δD, we compare total-column δD simulated with LMDZ and total-column δD obtained after the full convolution.

2 Applying averaging kernels to model outputs

This section recalls how we calculate convolved total-column δD (δD_{conv}) based on simulated raw total-column δD (δD_{raw}).

2.1 For TES

δD_{conv} is calculated by integrating convolved HDO and H_2O profiles over the vertical. For any given level i, convolved HDO/H_2O ratio is calculated as follows ([Worden et al., 2006]):

$$ln(R_{conv,i}) = ln(R_{p,i}) + \sum_{k=1}^{n} \left((A_{HH,ik} - A_{HD,ik}) \cdot ln\left(\frac{R_{raw,k}}{R_{p,k}}\right) + (A_{DD,ik} - A_{HD,ik} - A_{HH,ik} + A_{DH,ik}) \cdot ln\left(\frac{q_{raw,k}}{q_{p,k}}\right) \right)$$

where:
$R_{conv,i}$ is the convolved HDO/H_2O ratio at level i,

$R_{p,i}$ is the a-priori HDO/H_2O ratio at level i,
$R_{raw,i}$ is the raw HDO/H_2O ratio simulated by LMDZ at level i,
$q_{conv,i}$ is the convolved specific humidity at level i,
$q_{p,i}$ is the a-priori specific humidity at level i,
$q_{raw,i}$ is the raw specific humidity simulated by LMDZ at level i,
$A_{HH,ik}$ is the averaging kernel for H_2O at levels i, k,
$A_{DD,ik}$ is the averaging kernel for HDO at levels i, k,
$A_{HD,ik}$ and $A_{DH,ik}$ are the cross averaging kernels at levels i, k.

Therefore, when applying averaging kernels to LMDZ outputs, the convolution effect ($\delta D_{conv} - \delta D_{raw}$) has two components:

1. the effect of the difference between the a-priori δD profile and the simulated δD profile. Since the δD a-priori profile is constant in space and time, this component impacts $\delta D_{conv} - \delta D_{raw}$, but also impact the expected difference between real and retrieved δD.

2. the effect of the difference between the a-priori humidity profile and the simulated humidity profile. Since the prior profile is taken from reanalyses, this component impacts $\delta D_{conv} - \delta D_{raw}$ and reflects mainly the humidity bias of LMDZ relatively to the reanalyses. In contrast, real specific humidity should be close to the reanalyses. Therefore, this component should have a limited effect on the expected difference between real and retrieved δD.

Assuming that the reanalyses capture correctly real specific humidity profiles, the second component may be neglected when estimating the effect of limited vertical resolution and a-priori constraints on retrieved δD. Therefore, to first order, this effect could be estimated by the difference between convolved total-column δD assuming correct humidity ($\delta D_{conv|q}$) and simulated raw total-column δD (δD_{raw}), where:

$$ln(R_{conv|q,i}) = ln(R_{p,i}) + \sum_{k=1}^{n} (A_{HH,ik} - A_{HD,ik}) \cdot ln\left(\frac{R_{raw,k}}{R_{p,k}}\right)$$

2.2 For GOSAT

δD_{conv} is calculated from the total-column H_2O and HDO:

$$W_{conv} = W_p + \sum_{k=1}^{n} A_{H,k} \cdot (w_{raw,k} - w_{p,k})$$

$$X_{conv} = X_p + \sum_{k=1}^{n} A_{H,k} \cdot (w_{raw,k} \cdot R_{raw,k} - w_{p,k} \cdot R_{p,k})$$

where
W_{conv} and X_{conv} are the convolved total-column H_2O and HDO,
W_p and X_p are the a-priori total-column H_2O and HDO,
$w_{p,k}$ and $x_{p,k}$ are the a-priori partial-column H_2O and HDO in the layer k,
$w_{raw,k}$ and $x_{raw,k}$ are the raw simulated partial-column H_2O and HDO in the layer k,
$A_{H,k}$ and $A_{D,k}$ are the averaging kernels for H_2O and HDO in the layer k.
As for TES, $\delta D_{conv|q}$ can be calculated assuming $w_{raw,k} = w_{p,k}$.

3 Effect of instrument sensitivity on retrieved total-column δD

To summarize:

1. $\delta D_{conv|q} - \delta D_{raw}$ estimates the effect of measurement sensitivity (limited vertical resolution and a-priori constraints) on retrieved total-column δD in reality, assuming that real specific humidity profiles are similar to those in the reanalyses.

2. $\delta D_{conv} - \delta D_{raw}$ estimates the effect of instrument sensitivity on retrieved total-column δD in the world of LMDZ, considering the specific humidity biases of LMDZ relatively to reanalyses.

Annual-mean values of these quantities are shown on figures 1 and 2 for TES and GOSAT respectively.

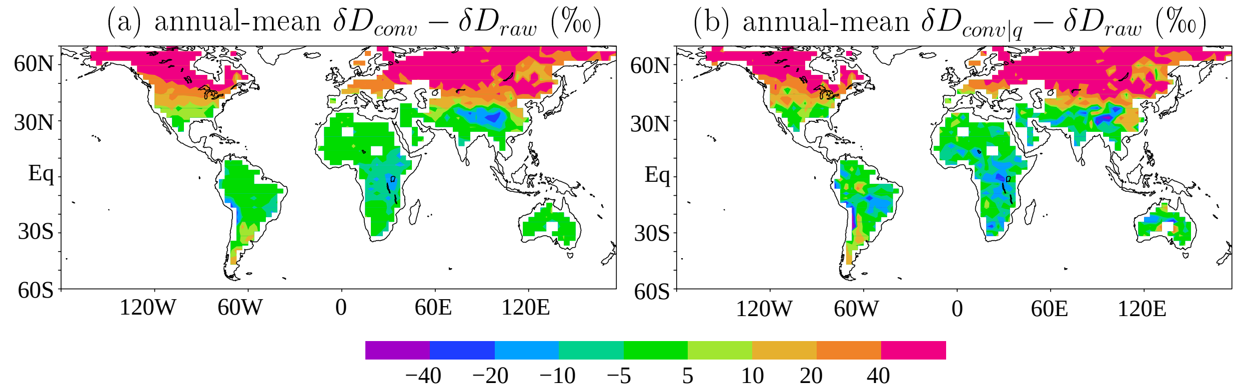

Figure 1: Effect of instrument sensitivity on annual-mean total-column δD retrieved by TES, considering $\delta D_{conv} - \delta D$ (a) and $\delta D_{conv|q} - \delta D_{raw}$ (b).

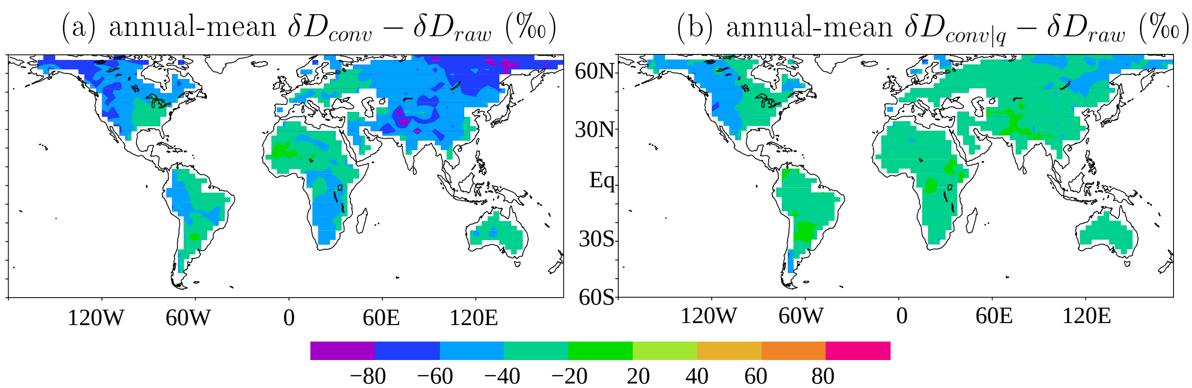

Figure 2: Same as 1 but for GOSAT.

3.1 For TES

The effect of the full convolution is to increase δD in mid and high latitudes. This is because in these regions, the a-priori δD profile has a larger impact on δD_{conv} and because the globally-constant a-priori δD profile is more enriched than δD_{raw}. In contrast in some tropical regions, the convolution decreases δD.

$\delta D_{conv} - \delta D_{raw}$ and $\delta D_{conv|q} - \delta D_{raw}$ are very similar, suggesting that simulated humidity biases have a small impact on the convolution. This suggests that in reality, the effect of instrument sensitivity is to increase retrieved δD in mid and high latitudes and to decrease it in some tropical regions.

3.2 For GOSAT

The effect of the full convolution is to decrease δD in many regions. However, when considering $\delta D_{conv|q} - \delta D_{raw}$, the effect is more restricted to high latitudes. This shows that the $\delta D_{conv} - \delta D_{raw}$ signal is mainly due to humidity biases in LMDZ. This suggests that in reality, the effect of instrument sensitivity is to decrease retrieved δD but that this effect is mainly restricted to high latitudes.

4 Correlation of this effect with precipitable water

The instrument sensitivity for δD may depend on the H_2O content of the atmosphere. To quantify this effect, we investigate the daily correlation between $\delta D_{conv} - \delta D_{raw}$ and precipitable water (W) and between $\delta D_{conv|q} - \delta D_{raw}$ and W.

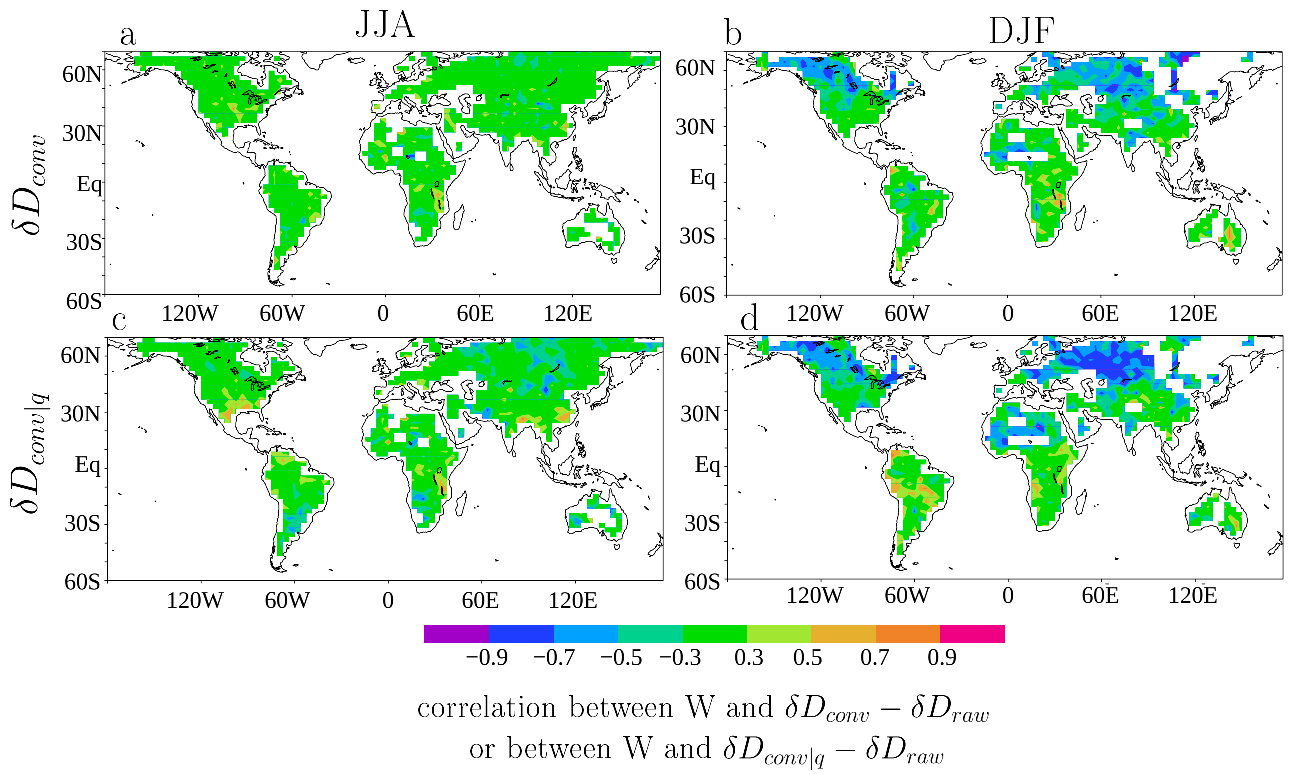

Figure 3: Daily correlation between $\delta D_{conv} - \delta D_{raw}$ and W (a,c) and between $\delta D_{conv|q} - \delta D_{raw}$ and W (b,d) in the TES data, for JJA (a,b) and DJF (c,d).

4.1 For TES

When W is lower, the sensitivity to δD is lower and so $\delta D_{conv} - \delta D_{raw}$ is larger. This explains the negative correlations (figure 3). This is especially the case in regions where W is low on average, i.e. over the Sahara and high latitudes.

$\delta D_{conv} - \delta D_{raw}$ and $\delta D_{conv|q} - \delta D_{raw}$ are very similar. This suggests that in reality, due to instrument sensitivity effects, retrieved δD is biased high on days when W is low.

4.2 For GOSAT

When W is lower, $\delta D_{conv} - \delta D_{raw}$ is also more negative in mid and high latitudes, over the Congo basin and over a large part of Asia. However, most of this effect is attenuated when considering $\delta D_{conv|q} - \delta D_{raw}$. This shows that the correlation between W and $\delta D_{conv} - \delta D_{raw}$ in LMDZ is mainly associated with simulated humidity biases.

This suggests that in reality, due to instrument sensitivity effects, retrieved δD is biased low on days when W is low, but this effect is relatively small.

5 Effect of instrument sensitivity on δD vs $ln(W)$ relationships

Since $\delta D_{conv} - \delta D_{raw}$ and $\delta D_{conv|q} - \delta D_{raw}$ correlate with W in some regions, this may have some impact on δD vs $ln(W)$ relationships. We investigate this impact by comparing δD vs $ln(W)$ relationships using δD_{raw}, $\delta D_{conv|q}$ and δD_{conv}.

5.1 For TES

The positive correlations between W and δD simulated by LMDZ become weaker when convolving by the averaging kernels (figure 5). Positive slopes become steeper (35% steeper on tropical average, table 1) and negative slopes also become steeper (120% steeper on tropical average) when convolving by averaging kernels (figure 6). The

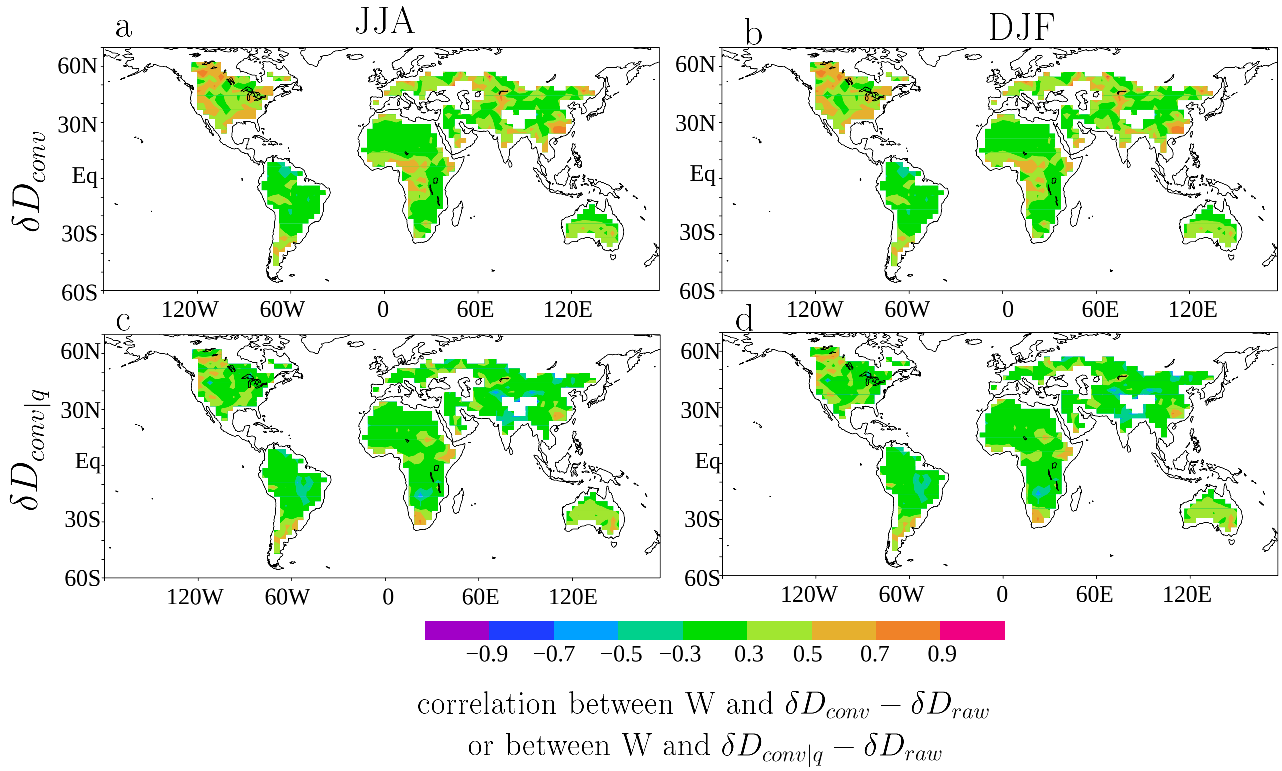

Figure 4: Same as figure 3 but for GOSAT.

amplification of negative slopes are consistent with figure 3 showing that when W is low, δD_{conv} is increased by the convolution.

When considering $\delta D_{conv|q}$, the correlations and slopes of the δD vs $ln(W)$ relationships are not affected much (table 1).

This suggests that the slopes of δD vs $ln(W)$ relationships are not systematically biased when observed by the TES data. When comparing LMDZ to TES, humidity biases in LMDZ lead convolved outputs to systematically overestimate positive slopes and underestimate negative slopes.

5.2 For GOSAT

The positive correlations between W and δD simulated by LMDZ become slightly weaker and the negative correlations disappear when convolving by averaging kernels (figure 7). However, positive slopes of the δD vs $ln(W)$ relationship become steeper (figure 8, 80% steeper on tropical average, table 1). The weaker correlations may be due the fact that the raw δD which correlates well with $ln(W)$ but the kernel convolution disrupts this raw δD. The larger slopes are consistent with figure 3 showing that when W is low, δD_{conv} is decreased.

Consistently with figure 4, there is little difference in correlations and in positive slopes when using $\delta D_{conv|q}$ or using δD_{raw}. There is just a slight weakening of negative slope (45% weaker on tropical average, table 1).

This suggests that the slopes of the δD vs $ln(W)$ relationships are not significantly biased when observed by GOSAT, except for a slight weakening of negative slopes. When comparing LMDZ to GOSAT, humidity biases in LMDZ lead convolved outputs to systematically overestimate positive slopes and underestimate negative slopes.

6 Conclusion

The effect of instrument sensitivity on the interpretation of observed δD-$ln(W)$ relationships and of model-data differences in these relationships is summarized in table 2.

References

[Worden et al., 2006] Worden, J., Bowman, K., Noone, D., Beer, R., Clough, S., Eldering, A., Fisher, B., Goldman, A., Gunson, M., Herman, R., Kulawik, S. S., Lampel, M., Luo, M., Osterman, G., Rinsland, C., Rodgers, C., Sander, S., Shephard, M., and Worden, H. (2006). Tropospheric Emission Spectrometer observations of the tropospheric HDO/H2O ratio: Estimation approach and characterization. *J. Geophy. Res.*, 111:D16309, doi:10.1029/2005JD006606.

[Worden et al., 2012] Worden, J., Wecht, K., Frankenberg, C., Alvarado, M., Bowman, K., Kort, E., Kulawik, S., Lee, M., Payne, V., and Worden, H. (2012). CH4 and CO distributions over tropical fires as observed by the Aura TES satellite instrument and modeled by GEOS-Chem. *Atmos. Chem. Phys. Discuss.*, 12:26207–26243.

instrument	δD considered	tropical mean	tropical-mean where slopes are positive	tropical-mean where slopes are negative
TES	δD_{raw}	0.24	0.39	-0.19
TES	δD_{conv}	0.10	0.52	-0.41
TES	$\delta D_{conv\|q}$	0.24	0.38	-0.15
GOSAT	δD_{raw}	0.06	0.44	-0.36
GOSAT	δD_{conv}	0.40	0.78	-0.42
GOSAT	$\delta D_{conv\|q}$	0.21	0.45	-0.20

Table 1: Tropical-mean values for δD vs $ln(W)$ slopes when considering δD_{raw} , δD_{conv} and $\delta D_{conv|q}$, for TES and for GOSAT. Note that these values are not directly comparable to table 3 in the main text because the mask was more stringent there.

instrument	Effect of measurement sensitivity (limited vertical resolution, a-priori constraints) on retrieved total column δD	Effect of model humidity biases on the model-data comparison
How the effect was estimated	We compare δD vs $ln(W)$ relationships derived from raw simulated δD (δD_{raw}) and from convolved δD assuming the simulated humidity profile equals the a-priori profile ($\delta D_{conv\|q}$)	We compare δD vs $ln(W)$ relationships derived from fully convolved δD (δD_{conv}) and from convolved δD assuming the simulated humidity profile equals the a-priori profile ($\delta D_{conv\|q}$)
TES	Observed δD vs $ln(W)$ relationships are not systematically biased when observed by the TES data	Humidity biases in LMDZ lead convolved outputs to systematically overestimate positive slopes and underestimate negative slopes.
GOSAT	Observed δD vs $ln(W)$ relationships are not significantly biased when observed by GOSAT, except for a slight weakening of negative slopes	Humidity biases in LMDZ lead convolved outputs to systematically overestimate positive slopes and underestimate negative slopes

Table 2: Summary of the effect of instrument sensitivity on δD vs $ln(W)$ relationships in the observations and for the model-data comparison, for TES and for GOSAT.

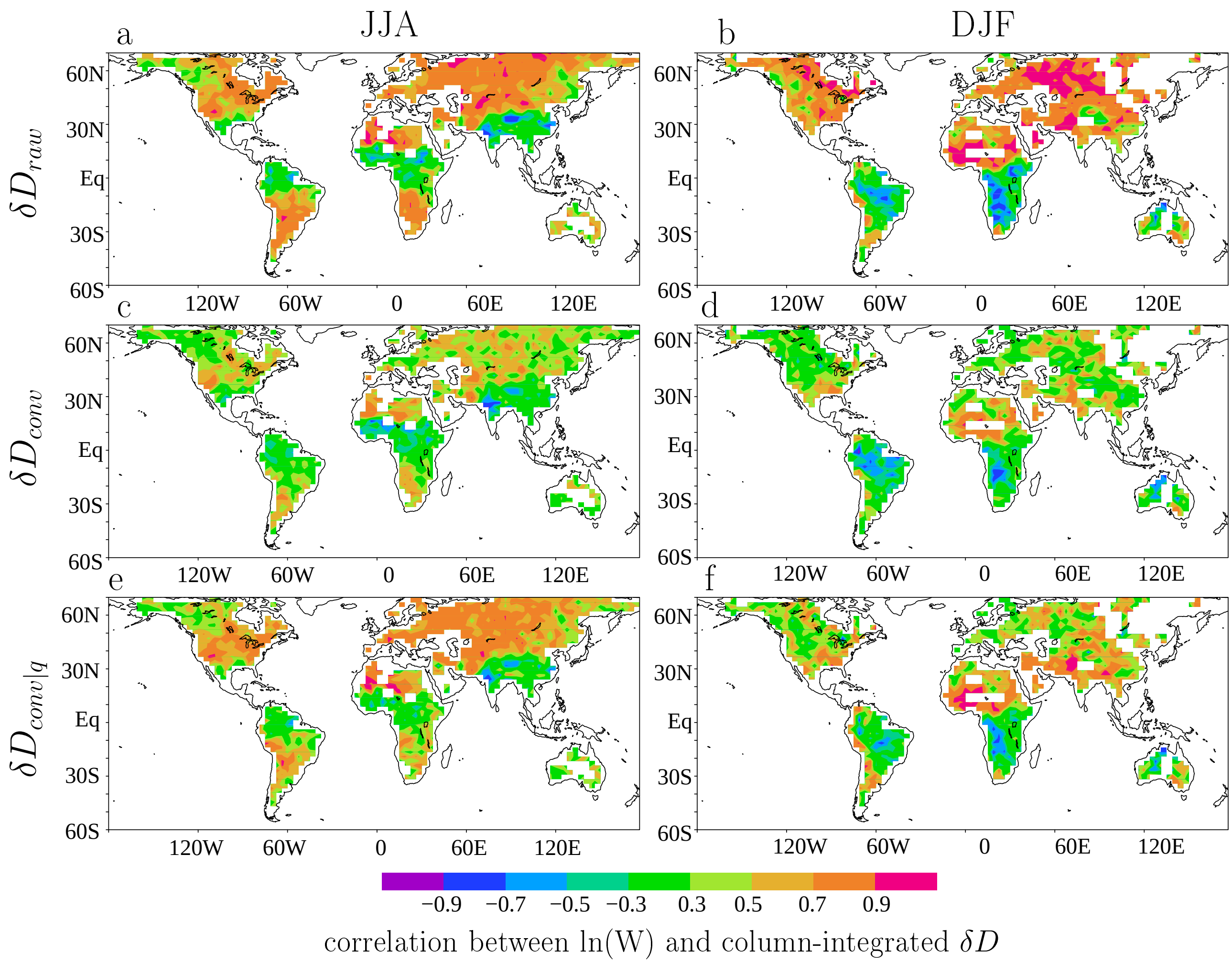

Figure 5: Effect of TES instrument sensitivity on δD vs $ln(W)$ relationships, by comparing the daily correlation between $ln(W)$ and δD when considering δD_{raw} (a-b), δD_{conv} (c-d) and $\delta D_{conv|q}$ (e-f), for JJA (left) and DJF (right).

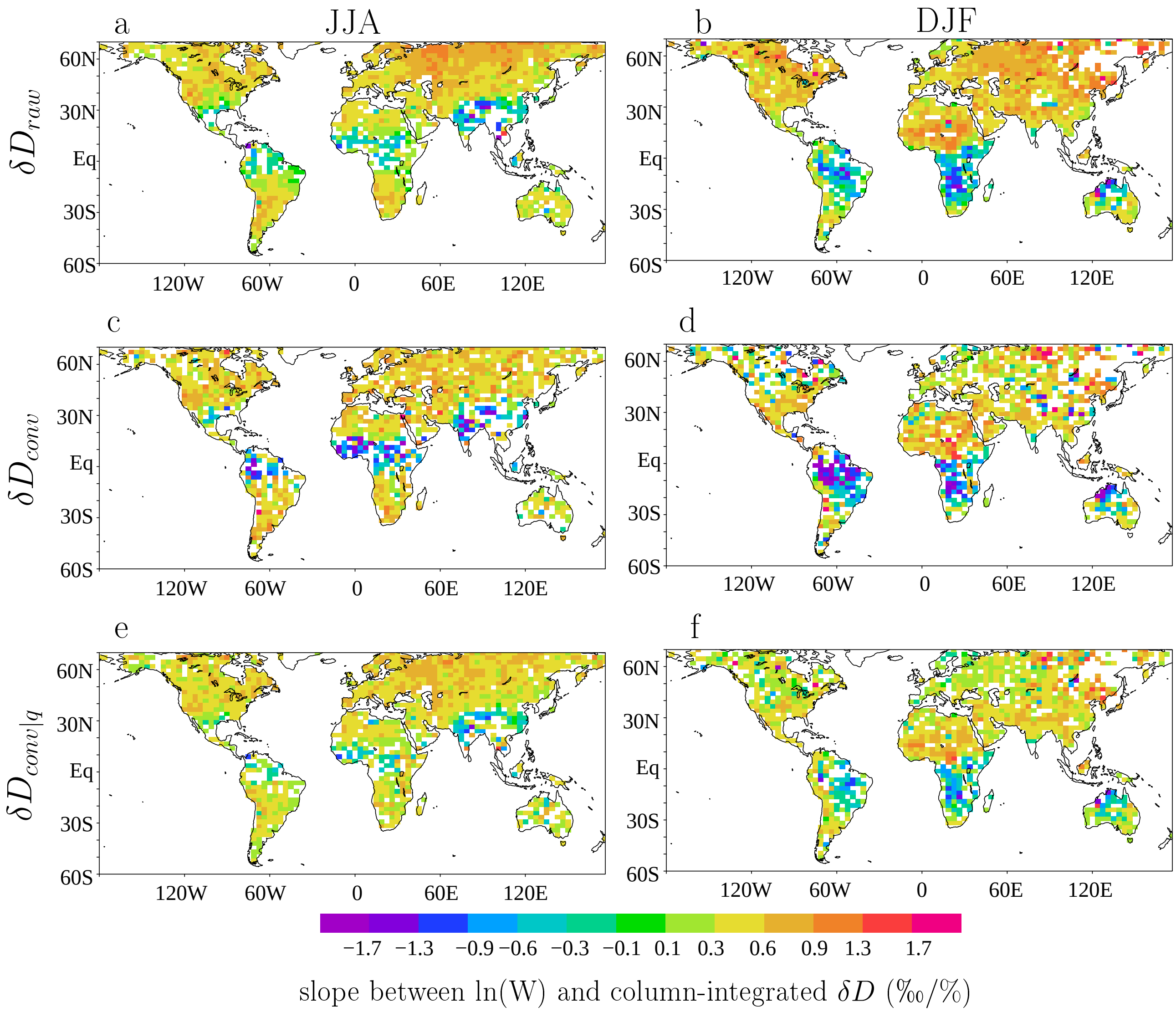

Figure 6: Same as figure 5 but for the δD vs $ln(W)$ slopes.

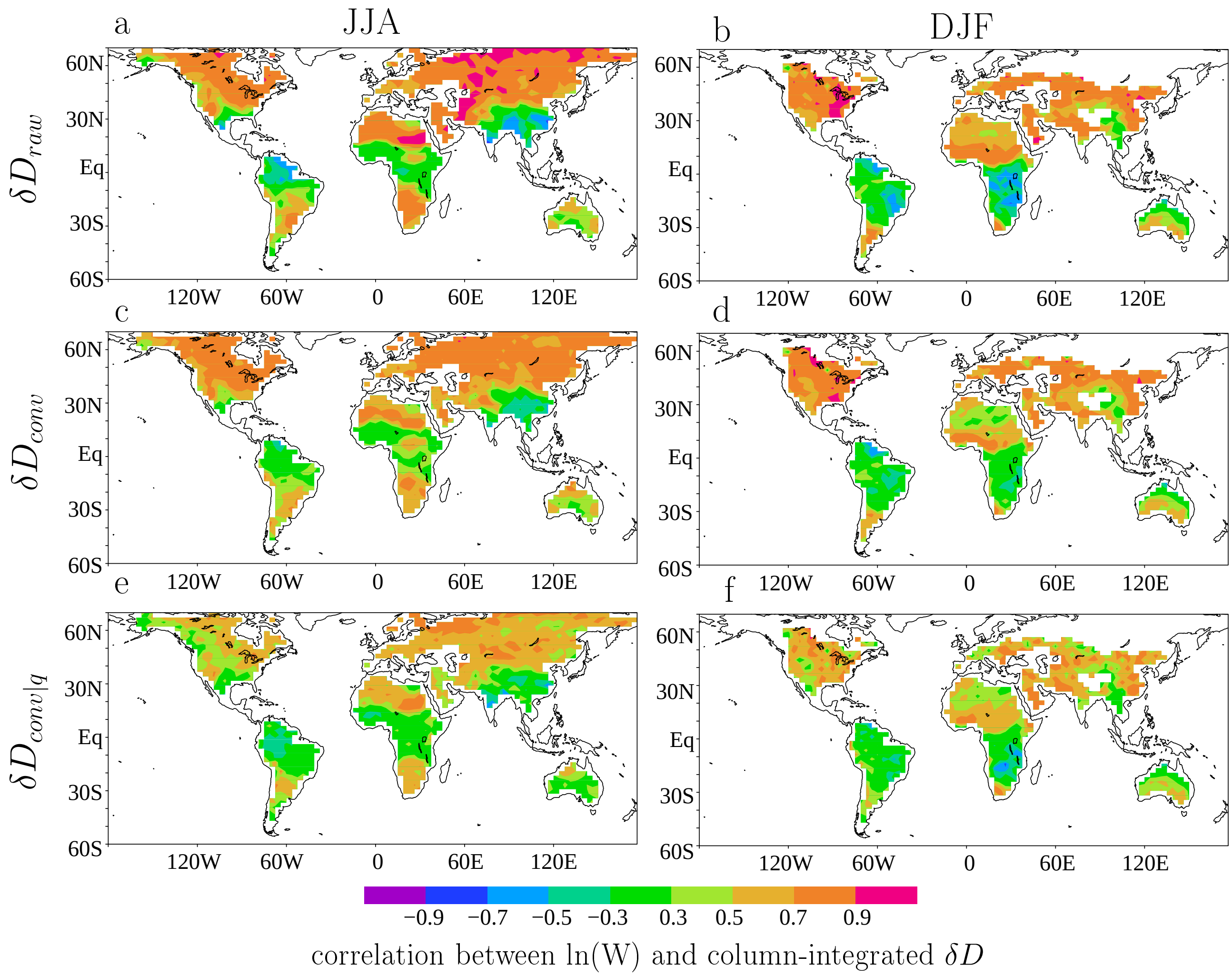

Figure 7: Same as figure 7 but for GOSAT

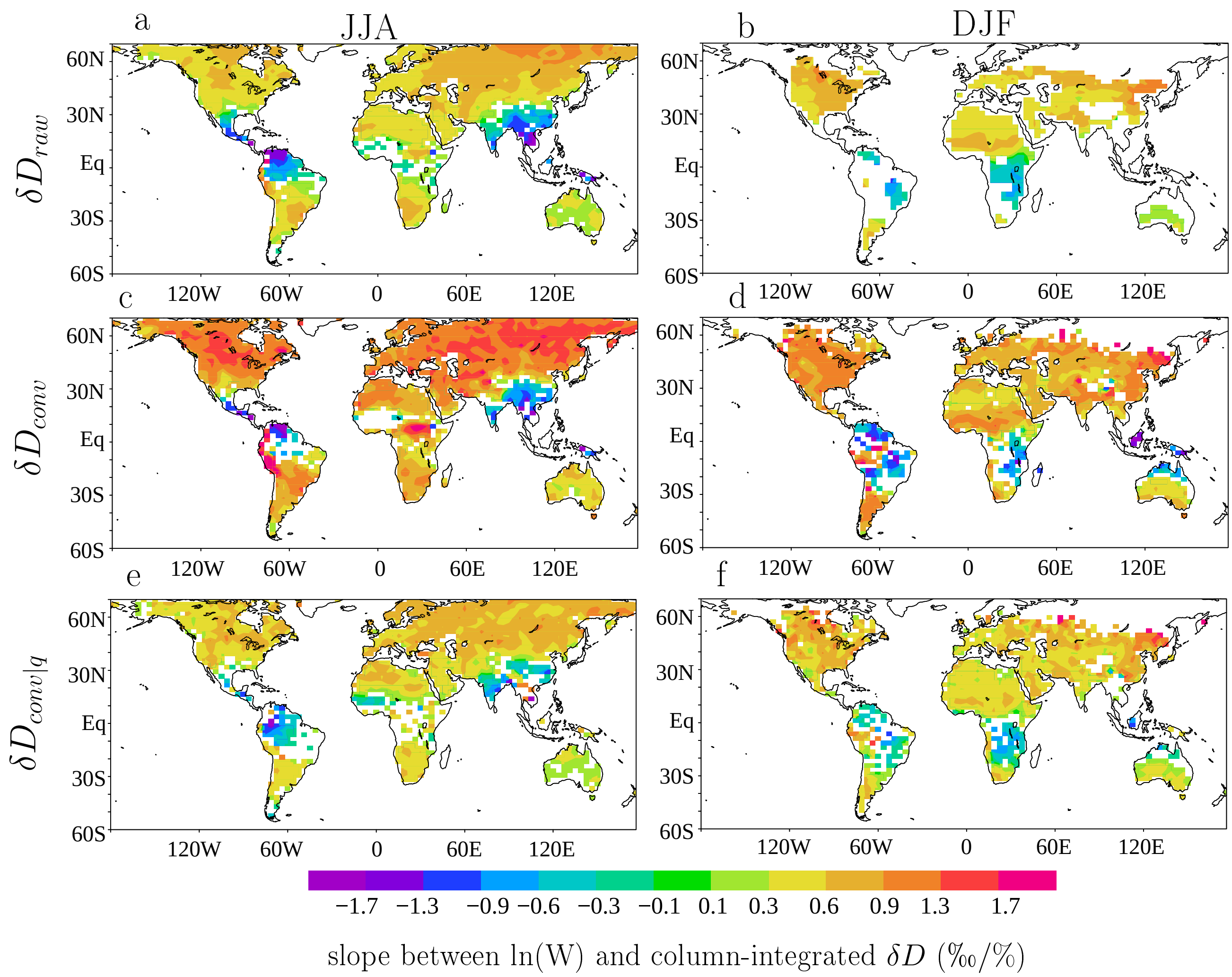

Figure 8: Same as figure 6 but for GOSAT.